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Doubly quasi-consistent parallel explicit peer methods with built-in global error estimation

G. Yu. Kulikov*and R. Weiner†

Abstract

Recently, Kulikov presented the idea of double quasi-consistency, which facilitates global error estimation and control, considerably. More precisely, a local error control implemented in such methods plays a part of the global error control at the same time. However, Kulikov studied only Nordsieck formulas and proved that there exists no doubly quasi-consistent scheme among those methods.

Here, we prove that the class of doubly quasi-consistent formulas is not empty and present the first example of such sort. This scheme belongs to the family of superconvergent explicit two-step peer methods constructed by Weiner, Schmitt, Podhaisky and Jebens. We present a sample of s-stage doubly quasi-consistent parallel explicit peer methods of order $s-1$ when $s=3$. The notion of embedded formulas is utilized to evaluate efficiently the local error of the constructed doubly quasi-consistent peer method and, hence, its global error at the same time. Numerical examples of this paper confirm clearly that the usual local error control implemented in doubly quasi-consistent numerical integration techniques is capable of producing numerical solutions for user-supplied accuracy conditions in automatic mode.

Keywords: doubly quasi-consistent numerical schemes, superconvergent explicit two-step peer methods, embedded formulas, adaptivity, local error estimation, automatic global error control.
AMS Subject Classification: 65L05, 65L06, 65L20, 65L50.

1 Introduction

Recently, Kulikov [7] presented a fruitful notion of quasi-consistent numerical integration of ordinary differential equations (ODEs) of the form

$$x'(t)=g\big(t,x(t)\big),\quad t\in[t_0,t_{end}],\quad x(t_0)=x^0 \tag{1}$$

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where $x(t) \in \mathbb{R}^m$ and $g : D \subset \mathbb{R}^{m+1} \to \mathbb{R}^m$ is a sufficiently smooth function. It implies merely an integration conducted by a quasi-consistent numerical scheme. The property of quasi-consistency goes back to 1976 (see [16]). Skeel discovered in the cited paper that the order of the global error of some numerical methods is equal to the order of their local error. Skeel and Jackson [19] explored consistency and quasi-consistency of Nordsieck formulas in 1977.

Later, Kulikov [7] studied advantages of quasi-consistent numerical integration by Nordsieck methods in the sense of global error estimation and control. He found that local error estimates of some quasi-consistent Nordsieck formulas can be sufficiently good approximations to the global error, at least for some ODEs. However, the usual quasi-consistency is not enough to ensure that the local error and the global error are asymptotically equal (i.e. they have the same principal term) for any problem. That is why he formulated a stronger property of double quasi-consistency for Nordsieck methods in [7], which means that the principal terms of the local and global errors coincide. Unfortunately, Kulikov proved in the cited paper that there exists no doubly quasi-consistent Nordsieck formula. The maximum that we can expect from conventional Nordsieck methods is the property of super-quasi-consistency discovered in [10]. On the other hand, it was predicted in [7] that doubly quasi-consistent numerical schemes can be found in the class of general linear methods, studied in [3] at length. Nevertheless, the issue of existence of such numerical formulas has still been open.

In this paper, we explore double quasi-consistency of explicit two-step peer methods introduced by Weiner et al. [22], which are a special family of general linear methods. When applied to problem (1) those numerical schemes read

$$x_{ki} = \sum_{j=1}^{s} b_{ij} x_{k-1,j} + \tau_k \sum_{j=1}^{s} a_{ij} g(t_{k-1,j}, x_{k-1,j}) + \tau_k \sum_{j=1}^{i-1} r_{ij} g(t_{kj}, x_{kj}) \tag{2}$$

where $t_{ki} := t_k + c_i\tau_k$, $i = 1, 2, \ldots, s$. The extra nodes t_{ki} of the integration mesh are fixed by the constants c_i. Method (2) can be easily represented in the matrix form

$$X_k = (B \otimes I_m) X_{k-1} + \tau_k (A \otimes I_m) g(T_{k-1}, X_{k-1}) + \tau_k (R \otimes I_m) g(T_k, X_k) \tag{3}$$

where I_m is the identity matrix of dimension m and $\otimes$ denotes the Kronecker tensor product (see, for example, [12]). Here, we have utilized the following notation:

$$T_k := (t_{ki})_{i=1}^{s}, \quad X_k := (x_{ki})_{i=1}^{s}, \quad g(T_k, X_k) := g(t_{ki}, x_{ki})_{i=1}^{s},$$

$$A := \left(a_{ij}\right)_{i,j=1}^{s}, \quad B := \left(b_{ij}\right)_{i,j=1}^{s}, \quad R := \left(r_{ij}\right)_{i,j=1}^{s}.$$

Notice that the matrix R is strictly lower triangular because method (3) is explicit. Moreover, these peer methods allow for a simple and convenient parallelization by setting $R = 0$. We will further restrict ourselves to this case.

The principal feature of peer methods is the fact that all entries of the solution vector X_k possess similar properties in terms of stability and accuracy of numerical integration. This means that any stage value of a peer method can be taken as the output solution.

Weiner et al. [23] discovered that some methods (2) are quasi-consistent. They used this property to boost the convergence order of the mentioned numerical schemes (further we call it the order of the method for the sake of brevity) and termed such formulas superconvergent two-step peer methods.

The goal of this paper is to study double quasi-consistency in the class of methods (2). In other words, we prove existence of doubly quasi-consistent numerical schemes and show their advantage for global error estimation and control. However, we further deal with the fixed-stepsize version of the explicit two-step peer methods. Therefore the stepsize $\tau_k = \tau$, below. This simplifies our search for doubly quasi-consistent explicit peer methods, significantly. Thus, consideration of only fixed-stepsize methods (2) corresponds well to the objective of this paper.

On the other hand, adaptivity can be incorporated into fixed-stepsize methods under discussion in the same way as it is done in geometric integration methods, i.e. we do not change the stepsize but rather use a time transformation of the problem under solution (see, for example, Chapter VIII in [4]). If it is efficient, we will utilize the arc-length parametrization, which does not require any a priori information of the solution, to transform equidistant meshes to variable ones that match the solution path. This transformation means that we merely replace ODE (1) with the equivalent problem

$$\frac{dt}{d\lambda} = \frac{1}{\sqrt{1 + \sum_{j=1}^{m} g_j^2\big(t(\lambda), x(\lambda)\big)}}, \qquad t(0) = t_0, \tag{4a}$$

$$\frac{dx_i}{d\lambda} = \frac{g_i\big(t(\lambda), x(\lambda)\big)}{\sqrt{1 + \sum_{j=1}^{m} g_j^2\big(t(\lambda), x(\lambda)\big)}}, \qquad x_i(0) = x_i^0, \quad i = 1, 2, \ldots, m, \tag{4b}$$

where λ is the new independent variable (the arc length of the solution curve) and the integer i stands for the index of an equation in system (1). It is known that the arc length parametrization possesses many attractive properties in numerical analysis (see, for example, [15]). Certainly, the length of the integration interval of time-transformed problem (4) is unknown a priori. Thus, we apply a Hermite interpolating polynomial of degree 5 to calculate the numerical solution at the end point t_{end} of the source problem (1).

To facilitate the local error estimation (and, hence, the global error evaluation as well) in methods (2) we exploit the notion of embedded formulas. However, embedded peer methods utilized for the error computation are of the same order in this paper. This is the principal distinction between our technique and what is usual in embedded Runge-Kutta formulas. The embedded methods presented here have only the local errors of different order. To our advantage, we do not need any higher order numerical solution to continue, for correctness of this error estimation. This means that we resolve the main inconsistency of the local error estimation by embedded method scheme where the error is evaluated for a lower order numerical solution but the actual integration is conducted by a higher order method whose error is unknown. We stress that the local error estimate of a doubly quasi-consistent scheme is an asymptotically accurate estimate to the global error

of the same method. This is a peculiar feature of any doubly quasi-consistent formula, by definition. Therefore we continue with the numerical solution calculated from the doubly quasi-consistent method in the pair of embedded peer formulas built below (see Sect. 3 for more details).

The remainder of this paper is organized as follows: In Section 2, we prove existence of doubly quasi-consistent peer methods in a constructive way. More precisely, we reformulate the definition of double quasi-consistency in terms of the coefficients of the explicit two-step peer methods and, then, give an instance of such schemes. Section 3 introduces embedded peer methods of the new sort. These methods can have the same classical order that facilitates significantly the local (and global) error estimation in the doubly quasi-consistent peer formula. An algorithm of global error control is also discussed there. Section 4 contains numerical tests that confirm the power of doubly quasi-consistent numerical schemes in the sense of efficiency of the global error estimation. The last section summarizes the results obtained in this paper and outlines future plans.

2 Existence of doubly quasi-consistent peer methods

First of all we introduce an equidistant mesh

$$w_\tau = \{t_k = t_0 + k\tau,\ k = 0, 1, \ldots, K,\ K\tau = t_{end} - t_0\}$$

with a stepsize τ on the integration segment $[t_0, t_{end}]$ and assume that ODE (1) has a unique solution $x(t)$ on the same interval. Then, we recall that parallel peer methods are to be explored here, i.e. $R = 0$ in formulas (2) and (3). Eventually, we arrive at the following s-stage numerical schemes to deal with:

$$x_{ki} = \sum_{j=1}^{s} b_{ij} x_{k-1,j} + \tau \sum_{j=1}^{s} a_{ij} g(t_{k-1,j}, x_{k-1,j}), \quad i = 1, 2, \ldots, s, \tag{5}$$

or in the matrix form

$$X_k = (B \otimes I_m) X_{k-1} + \tau (A \otimes I_m) g(T_{k-1}, X_{k-1}). \tag{6}$$

These explicit peer methods admit the parallel implementation when one processor is assigned to compute one stage value x_{ki} in a step of numerical integration.

Further, we follow Weiner et al. [22] to define consistency conditions and to present convergence results for explicit peer methods (5). We start with the definition of the defect of this method.

Definition 1 *The vector-function* $L(T_k, x(t), \tau) := \big(L_i(t_{ki}, x(t), \tau)\big)_{i=1}^{s}$ *where the entries satisfy*

$$L_i(t_{ki}, x(t), \tau) := x(t_{ki}) - \sum_{j=1}^{s} \Big(b_{ij} x(t_{k-1,j}) + \tau a_{ij} g\big(t_{k-1,j}, x(t_{k-1,j})\big) \Big) \tag{7}$$

is referred to as the defect of the explicit peer method (5).

Formula (7) is derived by substitution of the exact solution $x(t)$ evaluated at the mesh points into numerical scheme (5). It is also referred to as the residual of this method in the cited paper.

We recall that all stage values of peer methods are equally important. Thus,

Definition 2 *The peer method* (5) *is consistent of order* p *if and only if the following order conditions hold:*

$$\mathcal{AB}_i(l) := c_i^l - \sum_{j=1}^{s} \big(b_{ij}(c_j - 1)^l + l\, a_{ij}(c_j - 1)^{l-1} \big) = 0,\ l = 0, 1, \ldots, p,\ i = 1, 2, \ldots, s. \quad (8)$$

Order conditions (8) are obtained by the Taylor expansion of the defect (7) around the grid point t_k. Notice that we use slightly different definitions of the defect and the order conditions of peer methods than those that were introduced in [22] and [23]. In addition, we require in this paper that no order condition $\mathcal{AB}_i(p+1) = 0$, $i = 1, 2, \ldots, s$, is satisfied for a peer method (6) of the consistency order p.

In other words, Definitions 1 and 2 imply that $L(T_k, x(t), \tau) = \mathcal{O}(\tau^{p+1})$. It is evident that the latter condition is sufficient for convergence of order p. Certainly, the property of zero-stability is necessary for that. In our case, it means that any power of the matrix B is bounded. So, it suffices to require that the spectral radius of this matrix does not exceed one, i.e. $\varrho(B) \leq 1$, and the eigenvalues of modulus one are simple. In what follows, we consider that all peer methods (5) satisfy the zero-stability condition.

However, the consistency of order p is not necessary for convergence of order p. Weiner et al. [23] found that some explicit peer methods require less consistency for that.

Definition 3 *The peer method* (6) *is quasi-consistent of order* p *if and only if the following conditions hold:*

$$\mathcal{AB}(l) = 0, \quad l = 0, 1, \ldots, p-1, \quad (9a)$$

$$B \cdot \mathcal{AB}(p) = 0, \quad (9b)$$

where the vector $\mathcal{AB}(l) := \big(\mathcal{AB}_i(l)\big)_{i=1}^{s}$.

Notice that the latter definition deals with the matrix form of explicit parallel two-step peer methods. Definition 3 corresponds well to the definition of quasi-consistency presented in [16].

Condition (9a) says that the consistency of order $p-1$ must be satisfied. Then, the p-th order consistency is replaced with the more relaxed condition (9b). Weiner et al. [23] used the quasi-consistency to facilitate their search for variable-stepsize explicit peer methods of higher orders. They also prove in the cited paper that the quasi-consistency of order p implies convergence of order p in the class of variable-stepsize peer methods (2). We stress that that convergence result is not covered by Skeel [16], who dealt with fixed-stepsize methods only.

Kulikov [7] introduces a stronger property of double quasi-consistency to benefit global error evaluation. However, he considered Nordsieck formulas in the mentioned paper. Now

we reformulate that property in terms of the coefficients of method (6). Recall that, by definition, double quasi-consistency means that the principal terms of the local and global errors of a doubly quasi-consistent scheme coincide. We also notice that the definitions of the local error and the defect are equivalent for any explicit numerical method. Therefore formula (7) represents the local error of the peer method (5) as well.

Theorem 1 *The peer method* (6) *of order* p *is doubly quasi-consistent if and only if its coefficients* a_{ij}, b_{ij} *and* c_i *satisfy the following conditions:*

$$\mathcal{AB}(l) = 0, \quad l = 0, 1, \ldots, p-1, \tag{10a}$$

$$B \cdot \mathcal{AB}(p) = 0, \tag{10b}$$

$$B \cdot \mathcal{AB}(p+1) = 0, \tag{10c}$$

$$A \cdot \mathcal{AB}(p) = 0. \tag{10d}$$

Proof. The method (6) is supposed to be of order p. This means that its local error must be of the same order at least, i.e. $L(T_k, x(t), \tau) = \mathcal{O}(\tau^p)$. Thus, condition (10a) holds. To prove the remaining conditions we have to consider the error recursion of the explicit peer method (6).

We start with the error of the i-th stage value of our method, given by formula (5). By definition, $\Delta x_{ki} := x(t_{ki}) - x_{ki}$. Having subtracted the method (5) from the defect (7) we obtain

$$\Delta x_{ki} = \sum_{j=1}^{s} b_{ij} \Delta x_{k-1,j} + \tau \sum_{j=1}^{s} a_{ij} \partial_x g(t_k, x(t_k)) \Delta x_{k-1,j} + L_i(t_{ki}, x(t), \tau) + \mathcal{O}(\tau^{p+2}) \tag{11}$$

where $\partial_x g(t_k, x(t_k))$ denotes the partial derivative (Jacobian) of the mapping g with respect to the second argument and evaluated at the point $(t_k, x(t_k))$. Notice that all Jacobians appearing in formula (11) have been expanded in Taylor series around the point $(t_k, x(t_k))$ with an accuracy of $\mathcal{O}(\tau)$. Then, we take the order of the peer method into account to yield the error equation (11).

Now we introduce the notation $\Delta X_{k-1} = (\Delta x_{k-1,1}^T, \ldots, \Delta x_{k-1,s}^T)^T$ to proceed in the matrix form

$$\Delta X_k = (B \otimes I_m) \Delta X_{k-1} + \tau (A \otimes \partial_x g(t_k, x(t_k))) \Delta X_{k-1} + L(T_k, x(t), \tau) + \mathcal{O}(\tau^{p+2}). \tag{12}$$

It is clear from (12) that the method (6) is doubly quasi-consistent if and only if

$$(B \otimes I_m) \Delta X_{k-1} + \tau (A \otimes \partial_x g(t_k, x(t_k))) \Delta X_{k-1} = \mathcal{O}(\tau^{p+1}) \tag{13}$$

at any mesh point t_k. Condition (13) is equivalent to

$$\big((B \otimes I_m) + \tau (A \otimes \partial_x g(t_k, x(t_k))) \big) L(T_{k-1}, x(t), \tau) = \mathcal{O}(\tau^{p+2}) \tag{14}$$

because the error ΔX_{k-1} includes also accumulation of the errors committed in all previous mesh nodes.

Consider an expression $(V \otimes \partial_x g(t_k, x(t_k)))\mathcal{AB}(l)$ where V is an arbitrary fixed matrix in the component-wise form:

$$v_{i1}\partial_x g(t_k, x(t_k))\mathcal{AB}_1(l) + \ldots + v_{is}\partial_x g(t_k, x(t_k))\mathcal{AB}_s(l) = \partial_x g(t_k, x(t_k)) \sum_{j=1}^{s} v_{ij}\mathcal{AB}_j(l). \quad (15)$$

Having expanded entries of the defect $L(T_{k-1}, x(t), \tau)$ in the Taylor series in powers of the stepsize τ at the point t_{k-1}, taken into account condition (10a) proved earlier, utilized formula (15) and dropped the Kronecker tensor product, we deduct that condition (14) is equivalent to formulas (10b), (10c) and (10d). The theorem is proved. ■

Remark 1. It is clear that the order condition $\mathcal{AB}_i(p) = 0$ must not hold for any stage value x_{ki} of a doubly quasi-consistent peer method (6) of order p. If the above-mentioned order condition is satisfied for all stage values of the method it will be of order $p+1$ because of condition (10c). On the other hand, no stage value must satisfy it because all of them possess the same properties in terms of accuracy and stability (by the above definition of the consistency order of peer methods considered in this paper).

Remark 2. It follows from Theorem 1 that all doubly quasi-consistent peer methods (6) belong to the class of quasi-consistent peer schemes (6) (compare (9) and (10)). Then, the technique presented in [23] for constructing quasi-consistent peer methods is also useful to look for doubly quasi-consistent formulas.

With the use of that technique, we yield the following doubly quasi-consistent explicit parallel two-step peer method (6) presented by its coefficients:

$$A = \begin{pmatrix} \frac{89}{144} & \frac{23}{48} & -\frac{5}{36} \\ -\frac{133}{144} & \frac{29}{48} & \frac{55}{36} \\ -\frac{37}{144} & \frac{41}{48} & \frac{10}{9} \end{pmatrix}, \quad B = \begin{pmatrix} \frac{11}{18} & \frac{1}{2} & -\frac{1}{9} \\ \frac{11}{18} & \frac{1}{2} & -\frac{1}{9} \\ \frac{11}{18} & \frac{1}{2} & -\frac{1}{9} \end{pmatrix}, \quad c = \begin{pmatrix} \frac{1}{4} \\ \frac{1}{2} \\ 1 \end{pmatrix}. \quad (16)$$

This is a 3-stage explicit parallel peer method of order 2. It suffices to substitute the coefficients A, B and c in formulas (10) to confirm its double quasi-consistency. It also can easily be checked that no order condition $\mathcal{AB}_i(2) = 0$ is satisfied for method (16). The double quasi-consistency of the above peer method is confirmed numerically in Sect. 4.

Thus, we have proved that doubly quasi-consistent numerical schemes do exist. Further, we intend to utilize this property for an efficient global error estimation and control.

3 Global error control in the doubly quasi-consistent peer method

First of all, we are interested in an effective global error estimation mechanism. It can be done in the doubly quasi-consistent peer method presented above via understanding that

the principal terms of its local and global errors coincide. Therefore we just need an efficient local error evaluation technique to yield an asymptotically correct estimate to the true error at any mesh point. The latter is achieved by utilizing the notion of embedded methods, that is usual in the area of local error estimation. However, pairs of embedded schemes constructed earlier are required to include numerical methods of different orders. This was necessary for the correct local error evaluation. In this paper, we exploit embedded formulas of the same classical order, but with the local errors of different orders. This means that the true error of the output numerical solution is monitored and controlled.

Having used an embedded peer method (6) with coefficients A_{emb}, B_{emb} and $c_{emb} = c$, we arrive at the error evaluation scheme of the form

$$\Delta_1 X_k = \big((B_{emb} - B) \otimes I_m\big) X_{k-1} + \tau \big((A_{emb} - A) \otimes I_m\big) g(T_{k-1}, X_{k-1}) \tag{17}$$

where $\Delta_1 X_k$ denotes the principal term of the true error of the doubly quasi-consistent peer method and X_{k-1} implies the numerical solution computed by the same peer method. Thus, the global error estimation formula (17) is cheap in practice because it is a linear combination of the values known from method (16). It is also worthwhile to notice that this new global error estimation strategy does not required any Jacobian evaluation, which is needed in many other global error estimation schemes (see, for instance, [1], [8], [9], [10], [11], [13], [17], [18], [21]). Certainly, evaluation of the Jacobian of ODEs is natural in implicit numerical methods and, hence, can be utilized effectively in global error estimation techniques. However, it is unacceptable in explicit numerical methods, which do not require any Jacobian computation.

Further, we impose conditions on the embedded peer method to ensure correctness of the error estimation (17).

Theorem 2 *Let the peer method* (6) *be doubly quasi-consistent and of order p. Then formula* (17) *computes the principal term of its true error at grid points if and only if the coefficients A_{emb}, B_{emb} and c of the embedded peer method satisfy the following conditions:*

$$\mathcal{AB}(l)_{emb} = 0, \quad l = 0, 1, \ldots, p, \tag{18a}$$

$$B_{emb} \cdot \mathcal{AB}(p) = 0 \tag{18b}$$

where the vectors $\mathcal{AB}(l)_{emb}$, $l = 0, 1, \ldots, p$, are calculated for the coefficients of the embedded formula (6) *and the vector $\mathcal{AB}(p)$ is evaluated for the coefficients of the doubly quasi-consistent peer method in the embedded pair.*

Proof. The doubly quasi-consistent method (6) is of order p. Then, formulas (10) establish that its local error is $\mathcal{O}(\tau^p)$. The embedded method error estimation technique requires the local error of the embedded peer method with the coefficients A_{emb}, B_{emb} and c to be at least one order more accurate. This means that the order conditions (18a) hold. We recall that the definitions of the local error and the defect of explicit peer methods (6) coincide.

Further, with use of the notation of Theorem 1 we convert the error estimation formula (17) to the following form:

$$\begin{aligned}
\Delta_1 X_k &= \big((B_{emb}-B)\otimes I_m\big)X_{k-1}+\tau\big((A_{emb}-A)\otimes I_m\big)g(T_{k-1},X_{k-1})\\
&= \big(B_{emb}\otimes I_m\big)\big(X_{k-1}-X(t_{k-1})+X(t_{k-1})\big)+\tau\big(A_{emb}\otimes I_m\big)\\
&\times \big(g(T_{k-1},X_{k-1})-g(T_{k-1},X(t_{k-1}))+g(T_{k-1},X(t_{k-1}))\big)\\
&- \big(B\otimes I_m\big)\big(X_{k-1}-X(t_{k-1})+X(t_{k-1})\big)-\tau\big(A\otimes I_m\big)\\
&\times \big(g(T_{k-1},X_{k-1})-g(T_{k-1},X(t_{k-1}))+g(T_{k-1},X(t_{k-1}))\big)\\
&= L(T_k,x(t),\tau)+\big((B_{emb}-B)\otimes I_m\big)\Delta X_{k-1}+\mathcal{O}(\tau^{p+1}).
\end{aligned} \tag{19}$$

Here, we have taken into account Definition 1 of the defect of peer methods (6), the order of the doubly quasi-consistent peer method assumed in this theorem and condition (18a) proved earlier for the embedded peer formula with the coefficients A_{emb}, B_{emb} and c.

We emphasize that the numerical solution X_{k-1} implies the solution obtained by the doubly quasi-consistent peer method. It is shown in the proof of Theorem 1 that the error of any doubly quasi-consistent peer scheme (6) of order p satisfies the condition

$$\Delta X_{k-1}=L(T_{k-1},x(t),\tau)+\mathcal{O}(\tau^{p+1}). \tag{20}$$

Then formula (17) will calculate correctly the principal term of the local error (and, hence, the principal term of the true error) of the doubly quasi-consistent peer method if and only if

$$\big((B_{emb}-B)\otimes I_m\big)L(T_{k-1},x(t),\tau)=\mathcal{O}(\tau^{p+1}) \tag{21}$$

at any mesh point. This follows from (19), (20) and the fact that $L(T_k,x(t),\tau)=\mathcal{O}(\tau^p)$. The same arguments as those in the proof of Theorem 1 and conditions (10) show that (21) is equivalent to formula (18b). The theorem is proved. ■

Remark 3. It is clear from Theorem 2 that the error estimation formula (17) is correct even for embedded explicit parallel two-step peer schemes of the same order as that of the doubly quasi-consistent peer method, provided that conditions (18) hold. This is an interesting implication of double quasi-consistency, which is impossible in embedded Runge-Kutta formulas. Certainly, our error evaluation technique (17) will work for any higher order embedded peer method if we continue with the higher order numerical solution and utilize this solution on the right-hand side of the error estimation formula.

Remark 4. In practice, we prefer to replace condition (18b) imposed on the coefficients of the embedded peer scheme with the simpler formula

$$B_{emb}=B. \tag{22}$$

This increases the accuracy of the error estimation (17). On the other hand, it is evident that the matrix B_{emb} determined by condition (22) satisfies Theorem 2. This follows from Theorem 1.

With the use of Theorem 2 and formula (22), the embedded peer method (6) for the doubly quasi-consistent peer scheme (16) is chosen to have the coefficients:

$$A_{emb} = \begin{pmatrix} -\frac{1}{18} & \frac{47}{96} & \frac{151}{288} \\ \frac{7}{18} & -\frac{35}{96} & \frac{341}{288} \\ \frac{58}{18} & -\frac{476}{96} & \frac{1069}{288} \end{pmatrix}, \quad B_{emb} = \begin{pmatrix} \frac{11}{18} & \frac{1}{2} & -\frac{1}{9} \\ \frac{11}{18} & \frac{1}{2} & -\frac{1}{9} \\ \frac{11}{18} & \frac{1}{2} & -\frac{1}{9} \end{pmatrix}, \quad c = \begin{pmatrix} \frac{1}{4} \\ \frac{1}{2} \\ 1 \end{pmatrix}. \qquad (23)$$

It is easy to check that the order conditions $\mathcal{AB}(l)_{emb} = 0$ hold when $l = 1, 2$. This means that the embedded formula (23) has the local error of $\mathcal{O}(\tau^3)$. Thus, formula (17) evaluates the principal term of the true error of method (16), correctly. On the other hand, it is not difficult to verify that the embedded method (23) is only of classical order 2 because the quasi-consistency conditions (9) of order 3 are not satisfied for this method.

For the global error control, we exploit the stepsize selection algorithm utilized for Nordsieck formulas in [7]:

Global Error Control

Step 0. Initially, we set $\tau := \tau_{int}$, $\tau_{int} \in (0, 1)$ and suppose that $t_0 + \tau_{int} \leq t_{end}$;
Step 1. $k := 0$;
Step 2. While $t_k < t_{end}$ do,
$t_{k+1} := t_k + \tau$, compute X_{k+1}, $\Delta_1 X_{k+1}$;
Step 3. If $\max\limits_k \|\Delta_1 X_{k+1}\| > \epsilon_g$,
then $\tau := \gamma\tau \left(\epsilon_g / \max\limits_k \|\Delta_1 X_{k+1}\|\right)^{1/p}$, go to *Step 1*;
else Stop.

Here, p is the order of the implemented doubly quasi-consistent scheme (it equals 2 for the peer method (16)), $\gamma \in (0, 1)$ is a usual safety factor (it equals 0.8 in all numerical experiments, below) and ϵ_g (tolerance) is the required accuracy of computation (this parameter is to be set by the user). We recall that only fixed-stepsize peer methods (6) are considered in this paper. So, the above algorithm controls the diameter τ of equidistant grids. Our intention is to confirm in practice that the error evaluation formula (17) gives us correct estimates to the true error, which suffice for producing numerical solutions for user-supplied accuracy conditions in automatic mode. In the next section, we present a number of numerical tests to support our global error estimation technique.

4 Numerical examples

To check the theoretical developments above, we solve numerically a number of problems with known exact solutions by the peer method (16) with the global error control algorithm presented at the end of Sect. 3. We want to confirm that the error estimation formula (17) is capable of producing asymptotically correct estimates to the global error of the doubly

quasi-consistent peer method. Such estimates are utilized in the mentioned global error control. We observe also the dynamical behaviour of the local and true errors of method (16) when it is applied to various test problems. Thus, we verify double quasi-consistency of our peer scheme in practice.

First of all we repeat numerical experiments conducted for Nordsieck formulas in [7], but now for the doubly quasi-consistent peer method (16). So, we begin with the following test problems:

$$x_1'(t) = 2t x_2^{1/5}(t) x_4(t), \quad x_2'(t) = 10t \exp\Big(5\big(x_3(t)-1\big)\Big) x_4(t), \tag{24a}$$

$$x_3'(t) = 2t x_4(t), \quad x_4'(t) = -2t \ln\big(x_1(t)\big) \tag{24b}$$

where $t \in [0,3]$ and $x(0) = (1,1,1,1)^T$;

$$x_1''(t) = x_1(t) + 2x_2'(t) - \mu_1 \frac{x_1(t)+\mu_2}{y_1(t)} - \mu_2 \frac{x_1(t)-\mu_1}{y_2(t)}, \tag{25a}$$

$$x_2''(t) = x_2(t) - 2x_1'(t) - \mu_1 \frac{x_2(t)}{y_1(t)} - \mu_2 \frac{x_2(t)}{y_2(t)}, \tag{25b}$$

$$y_1(t) = \Big((x_1(t)+\mu_2)^2 + x_2^2(t)\Big)^{3/2}, \; y_2(t) = \Big((x_1(t)-\mu_1)^2 + x_2^2(t)\Big)^{3/2} \tag{25c}$$

where $t \in [0,T]$, $T = 17.065216560157962558891$, $\mu_1 = 1-\mu_2$ and $\mu_2 = 0.012277471$. The initial values of problem (25) are: $x_1(0) = 0.994$, $x_1'(0) = 0$, $x_2(0) = 0$, $x_2'(0) = -2.00158510637908252240$. We stress that the integration interval of the first problem has been increased significantly and that makes it more difficult for the global error control. For example, our numerical experiments show that the extended quasi-consistent Nordsieck formulas introduced in [7] fail to solve this problem for user-supplied accuracy conditions in automatic mode. It is not surprising because those numerical schemes are not doubly quasi-consistent and, hence, the new global error control concept is not expected to work successfully in the extended Nordsieck methods for any ODE.

Problem (24) has the exact solution

$$x_1(t) = \exp\big(\sin t^2\big), \quad x_2(t) = \exp\big(5\sin t^2\big), \quad x_3(t) = \sin t^2 + 1, \quad x_4(t) = \cos t^2. \tag{26}$$

Therefore we can calculate exact errors of numerical integrations and compare them with prescribed tolerances ϵ_g. In this way, we check how the error estimation formula (17) and the global error control mechanism work in the doubly quasi-consistent peer method presented in Sect. 2. Problem (25) has no analytic solution, but it is still useful to gain experience because its solution-path is periodic with the period T (this solution is called the Arenstorf orbit, see [5, p. 129, 130] for more details). Thus, we merely monitor the error at the point T to verify the quality of numerical solutions computed.

Kulikov [7] found that it is efficient to solve problem (24) in its original form and to apply the arc-length parametrization (4) to ODE (25). Here, we use only the most efficient way to integrate test problems numerically. All codes are written in `MATLAB 6.5.1` and

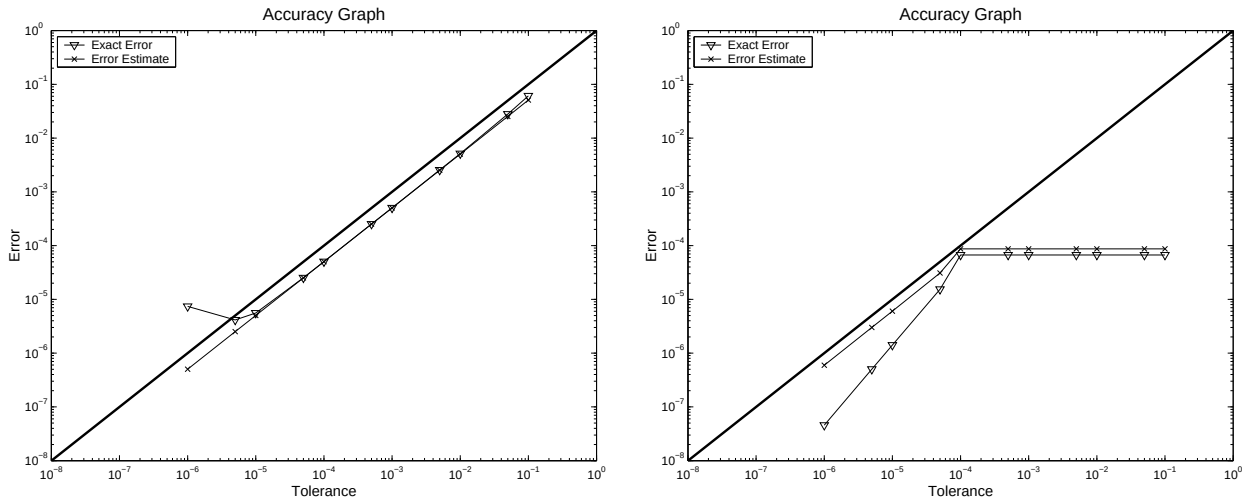

Figure 1: Test results for problem (24) solved in the original form (the left-hand graph) and for problem (25) solved in the time-transformed form (4) (the right-hand graph).

run on a personal computer with processor `Intel Pentium IV, 3.0 GHz` under operating system `MICROSOFT WINDOWS XP`.

The initial stepsize τ_{int} is chosen to be 0.01 in most tests of this paper. Notice that method (16) is two-step. Thus, a starting procedure of good quality is required. We apply formulas of the exact solution to calculate x_{01}, x_{02} and x_{03}, where they are available. For example, the exact solution (26) is used to start numerical integrations for test problem (24). Otherwise, we use the extrapolated Mid-Point Rule, as explained in [7], to calculate these stage values numerically and consider that the initial error does not influence experimental data, dramatically. The stage value x_{k3} is taken as the output solution at any mesh point t_{k+1}.

Fig. 1 displays the behaviour of the global error and its estimate computed by (17) for a set number of tolerances ϵ_g. Here and below, the error and the estimate have been plotted on the graphs scaled logarithmically in sup-norm. We see that almost all numerical solutions have been calculated for the specified accuracy conditions for both test ODEs, i.e the global errors are below the thick line representing our accuracy requirements. Certainly, round-off errors can influence the accuracy of numerical integration when the stepsize is sufficiently small, i.e. when we use the most stringent tolerances. This test says clearly that the error evaluation formula (17) produces accurate estimates to the global error, which, then, are utilized effectively in the global error control algorithm.

Fig. 2 and 3 exhibit the dynamical behaviour of the true error, the error estimated by formula (17) and the local error for ODEs (24) and (25), respectively. We have utilized the formulas of exact solution (26) to evaluate precisely the local and true errors for the first test problem. The second test problem has no exact solution in closed form. So, we

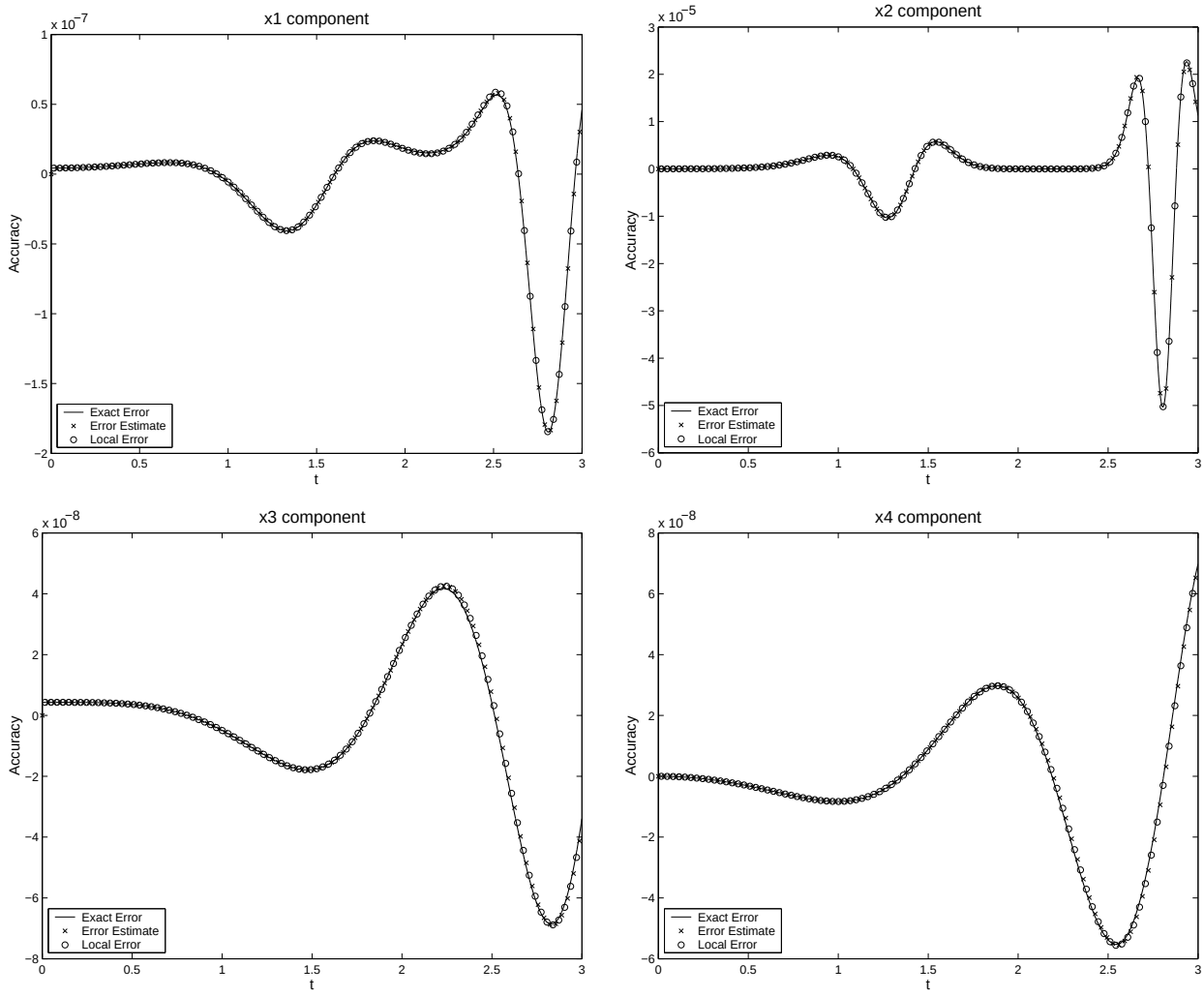

Figure 2: The exact error, the error estimated by formula (17) and the local error of method (16) applied to problem (24).

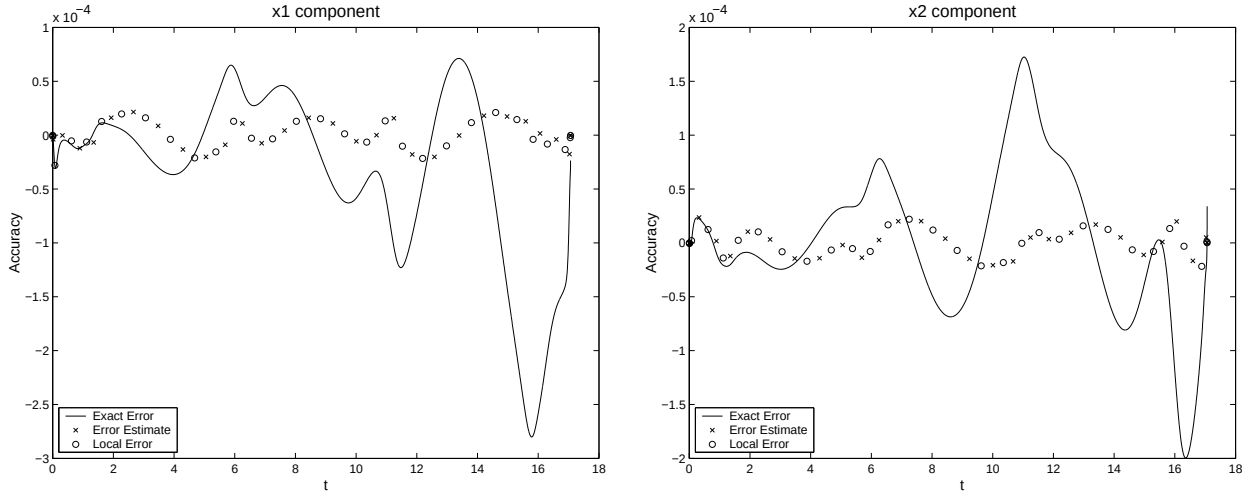

Figure 3: The exact error, the error estimated by formula (17) and the local error of method (16) applied to the time-transformed problem (25).

have applied the following 3-stage explicit parallel peer method of order 3:

$$A_{ref} = \begin{pmatrix} \frac{1}{9} & -\frac{11}{48} & \frac{53}{144} \\ \frac{5}{9} & -\frac{13}{12} & \frac{37}{36} \\ \frac{28}{9} & -\frac{17}{3} & \frac{32}{9} \end{pmatrix}, \quad B_{ref} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix}, \quad c = \begin{pmatrix} \frac{1}{4} \\ \frac{1}{2} \\ 1 \end{pmatrix}$$

to calculate the reference solution at the grid nodes. The grid is fixed in advance by the global error control algorithm for $\epsilon_g := 10^{-4}$. However, we reduce the number of plotted points for the local error and the error estimate to make them clearly marked in all figures showing the dynamical behaviour. Moreover, we are forced to use nonintersecting sets of plotted nodes for these quantites. Otherwise, their symbols will not be distinguishable on the majority of figures in this paper.

These data show that the local and true errors of the numerical solutions behave similarly. More precisely, they coincide for ODE (24) and differ slightly for ODE (25). This is exactly what we expect from any doubly quasi-consistent numerical scheme. In addition, the error estimates computed by formula (17) approximate both errors with high accuracy. However, we have to keep in mind that double quasi-consistency ensures that only the principal terms of the local and true errors coincide. Remaining terms of these errors can differ considerably. This means that magnitudes of the local and true errors will be close if the stepsize τ is sufficiently small and/or the integration interval $[t_0, t_{end}]$ is short enough. That is why the picture is slightly worse for the second test problem. We have also to remark that the reference solution utilized for the computation of the above-mentioned errors might not be accurate enough to produce good quality results for this ODE. On the other hand, the differences between the local error, the true error and the error estimate are small enough and do not influence essentially the performance of the global error control

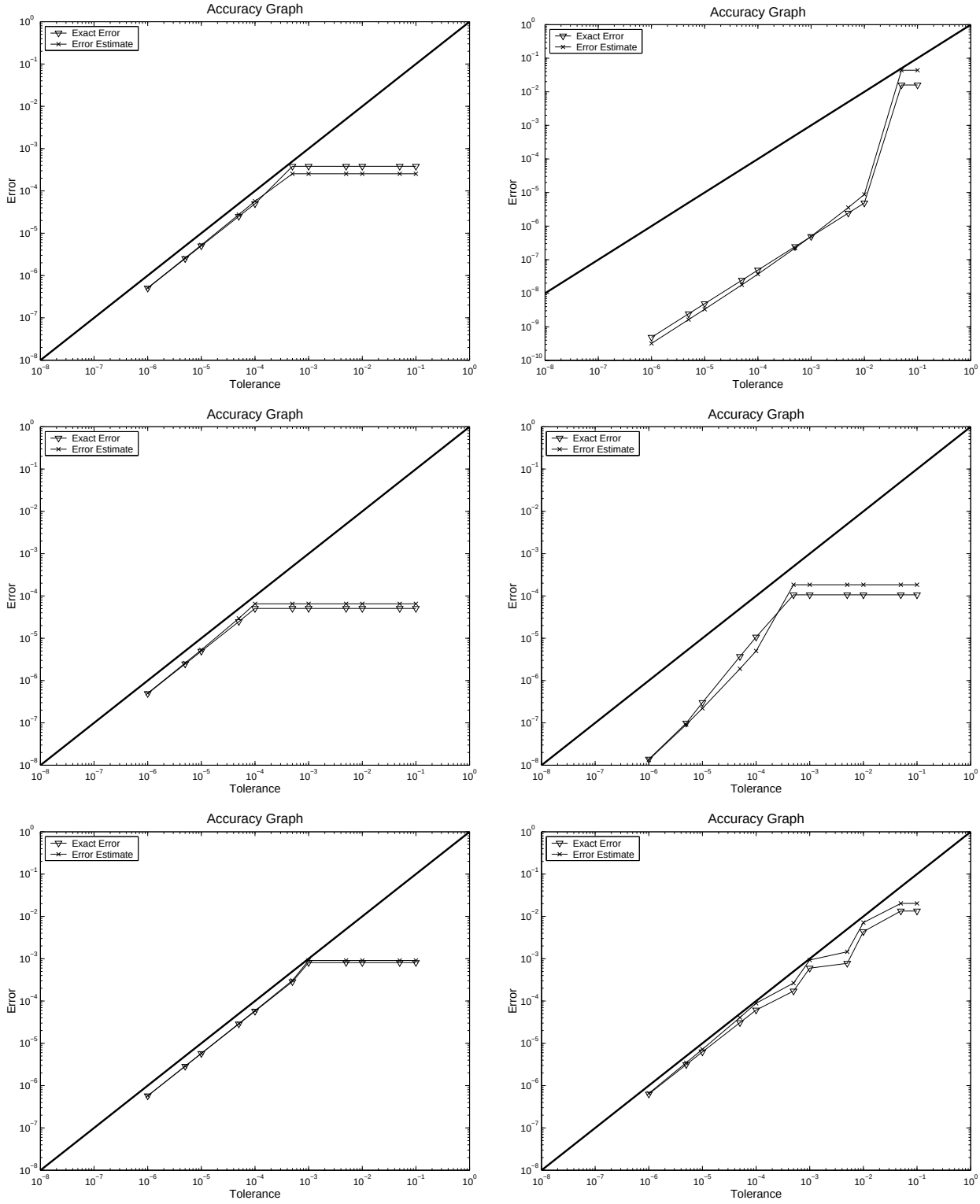

Figure 4: Test results for the nonstiff problems (27), (28), (29) in the original form (the left-hand graphs) and for the same but mildly stiff problems solved in the time-transformed form (4) (the right-hand graphs).

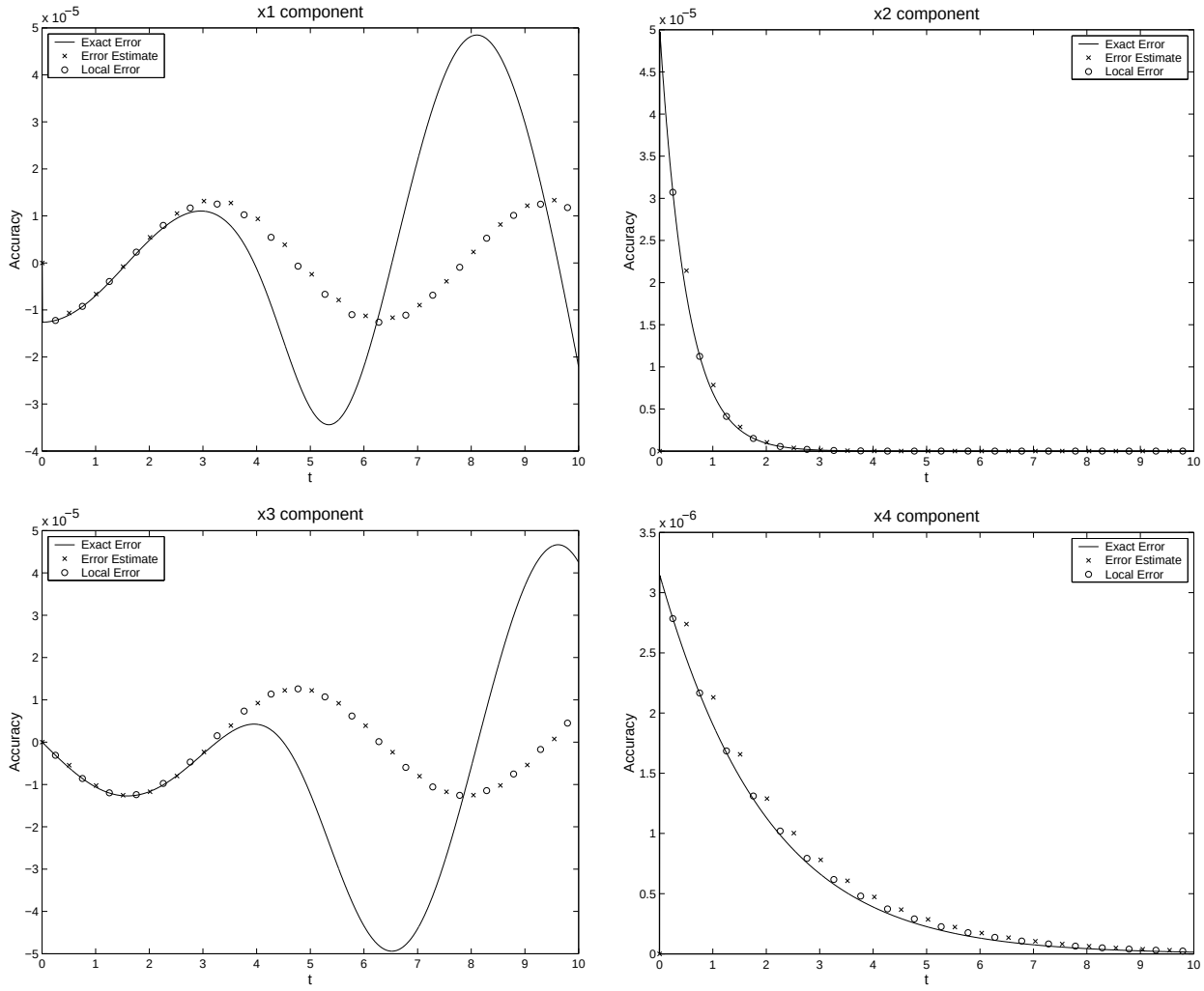

Figure 5: The exact error, the error estimated by formula (17) and the local error of method (16) applied to the nonstiff problem (27).

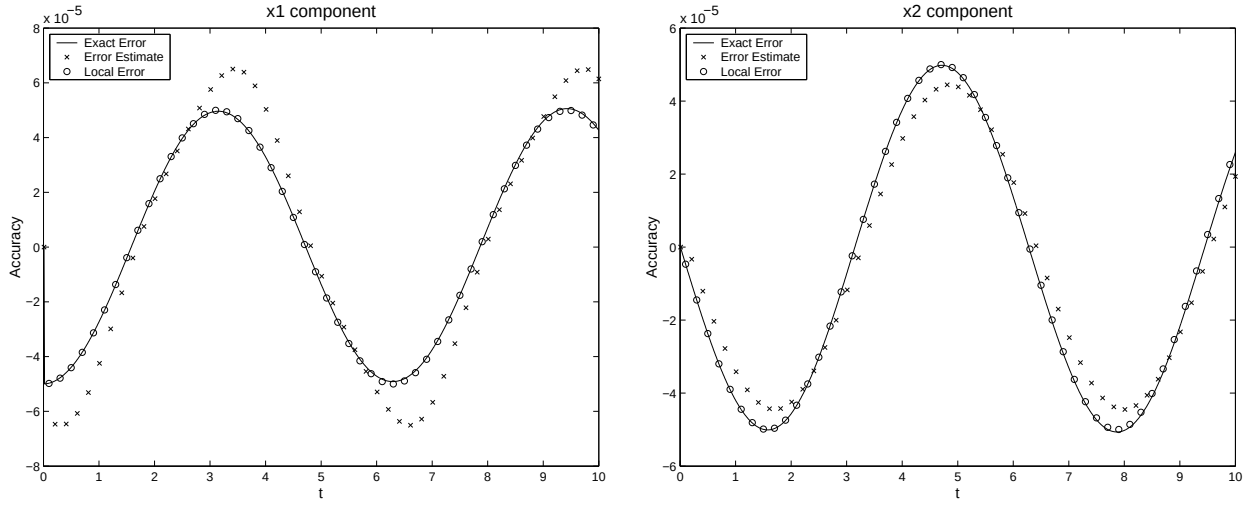

Figure 6: The exact error, the error estimated by formula (17) and the local error of method (16) applied to the nonstiff problem (28).

mechanism for ODE (25) (see the right-hand graph in Fig. 1). Nevertheless, we want to conduct more numerical experiments to gain confidence in the conclusion made.

Further, we test our doubly quasi-consistent peer method on three problems that can be potentially stiff. They are:

$$x_1'(t) = \mu\big(x_4^4(t)/x_2(t) - x_1^2(t) - x_3^2(t)\big) - x_3(t), \tag{27a}$$

$$x_2'(t) = \mu\big(x_4^4(t) - x_2(t)\big) - 2x_2(t), x_3'(t) = x_1(t), x_4'(t) = -x_2^{1/4}(t)/2 \tag{27b}$$

where $t \in [0, 10]$ and $x(0) = (1, 1, 0, 1)^T$;

$$x_1'(t) = \mu\big(\cos^2(t)\sin(t) + 2\cos(t) - (2 + x_1(t)x_2(t))x_1(t)\big) - x_2(t), \tag{28a}$$

$$x_2'(t) = x_1(t) + x_2(t) - \sin(t) \tag{28b}$$

where $t \in [0, 10]$ and $x(0) = (1, 0)^T$;

$$x_1'(t) = \mu\big(\sin(4t) - x_1(t)\big) + 4\cos(4t) \tag{29}$$

where $t \in [0, 10]$ and $x_1(0) = 1$. The exact solutions of these problems are:

- for ODE (27)

$$x_1(t) = \cos t, \quad x_2(t) = \exp(-2t), \quad x_3(t) = \sin t, \quad x_4(t) = \exp(-0.5t); \tag{30}$$

- for ODE (28)

$$x_1(t) = \cos t, \quad x_2(t) = \sin t; \tag{31}$$

- for ODE (29)

$$x_1(t) = \exp(-\mu t) + \sin(4t). \tag{32}$$

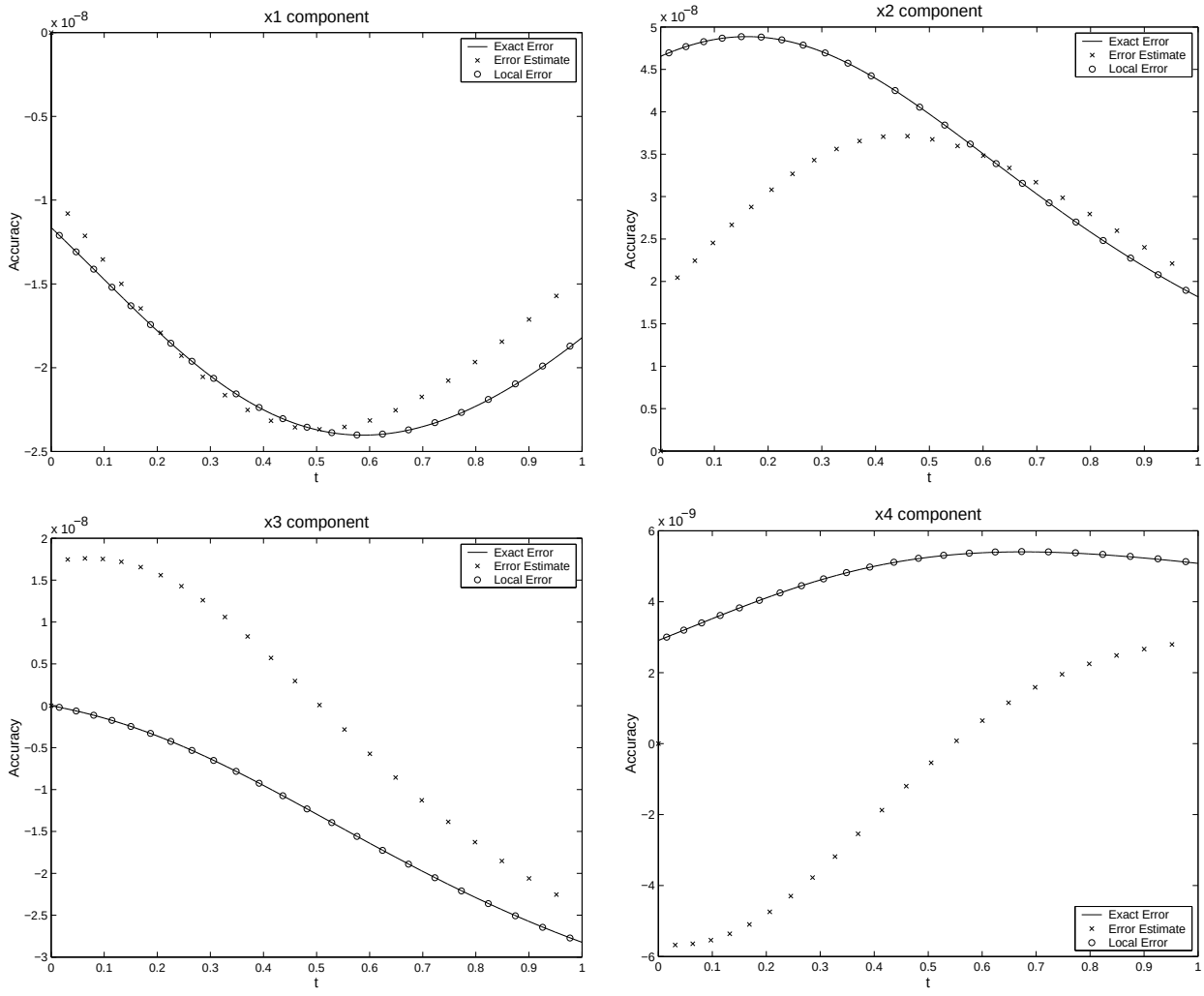

Figure 7: The exact error, the error estimated by formula (17) and the local error of method (16) applied to the time-transformed mildly stiff problem (27).

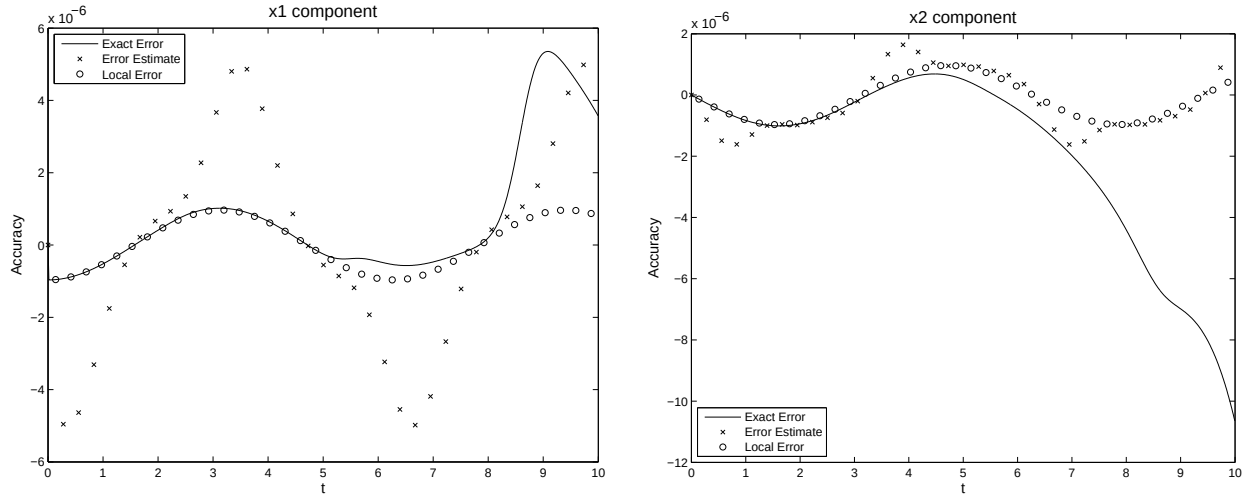

Figure 8: The exact error, the error estimated by formula (17) and the local error of method (16) applied to the time-transformed mildly stiff problem (28).

The last test problem is of Prothero and Robinson's type (see [14]). The parameter μ determines the stiffness of problems (27), (28) and (29). We examine two regimes: the nonstiff regime $\mu = 1$ and the mildly stiff regime $\mu = 100$. All the nonstiff problems are solved on the interval $[0, 10]$. The corresponding mildly stiff problems are integrated on the same intervals, except for the first one. The mildly stiff problem (27) is solved on the integration segments $[0, 1]$. The exact solutions (30), (31) and (32) are used to calculate the global errors of numerical solutions in Fig. 4 and the local and true errors in Fig. 5–9.

The results of this experiment say that the error estimation formula (17) works perfectly. It allows the global errors to be controlled effectively by the algorithm presented at the end of Sect. 3. Our doubly quasi-consistent peer method (16) with the global error control is capable of producing numerical solutions for a variety of tolerances chosen in the test and for both the nonstiff problems and the mildly stiff ones. All the numerical solutions are computed for the specified accuracy conditions in automatic mode.

Fig. 5–9 show the local error, the true error and the error estimate of the numerical solutions in dynamics when $\epsilon_g := 10^{-4}$. Usually, these quantities coincide (or they are very close, if we take into account the scales of the pictures). We must also keep in mind that the local errors and the error estimates are plotted in different time points. However, the local and true errors are slightly different for two components in Fig. 5. This can be easily explained by the length of the integration interval and the imposed accuracy condition. On the other hand, the distances between these errors and the error estimate do not exceed the required accuracy of the computation, i.e. $\epsilon_g := 10^{-4}$. This is exactly what is expected from the global error control mechanism.

Thus, our numerical examples confirm clearly existence and importance of doubly quasi-consistent numerical schemes in practice.

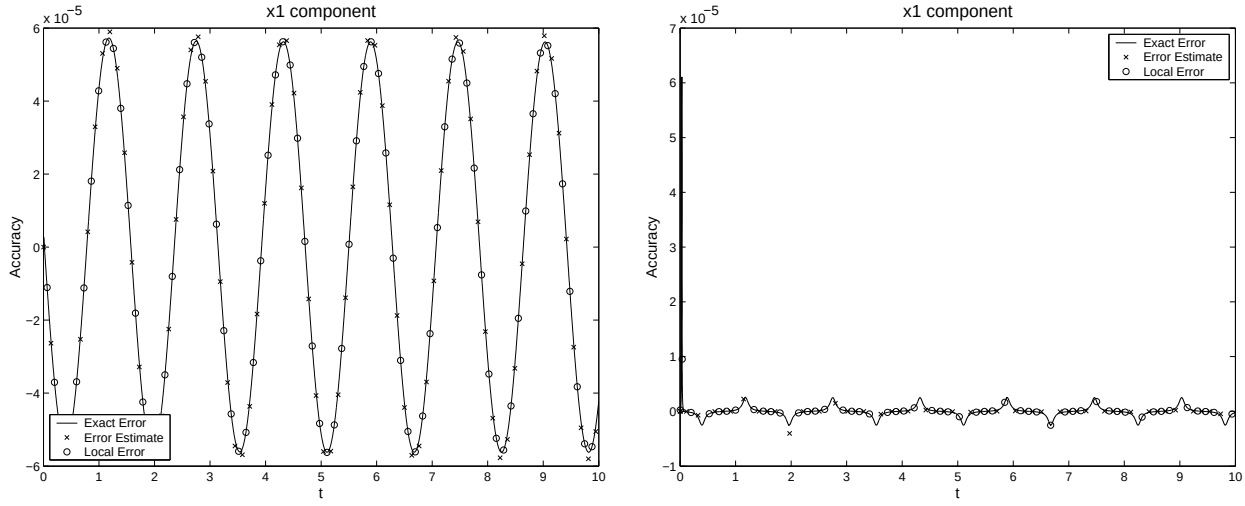

Figure 9: The exact error, the error estimated by formula (17) and the local error of method (16) applied to the nonstiff problem (29) (the left-hand graph) the time-transformed mildly stiff problem (29) (the right-hand graph).

5 Conclusion

This paper is the first practical contribution to the realm of doubly quasi-consistent numerical schemes. We point out that Kulikov [7] introduced the notion of double quasi-consistency and predicted existence of doubly quasi-consistent formulas among general linear methods, but did not present any sample of such techniques. Here, we have reformulated his property of double quasi-consistency in the form of the algebraic conditions imposed on the coefficients of parallel explicit two-step peer methods (see Theorem 1) and have proved that the class of doubly quasi-consistent numerical schemes is not empty. This paper has also confirmed that the new idea of global error control introduced in the cited paper works perfectly in doubly quasi-consistent formulas.

We have extended the embedded method error estimation technique to numerical schemes of the same convergence order. Most importantly, we have resolved the main inconsistency of the local error estimation by embedded method approach where the error is evaluated for a lower order numerical solution but the actual integration is conducted by a higher order method whose error is unknown. We evaluate the error of the output numerical solution in our pair of embedded peer methods (see Sect. 3).

Certainly, this paper is mainly of theoretical interest despite the good numerical results. The principal reason is that the fixed-stepsize integration is not efficient in practice. The arc-length parametrization improves the situation with the fixed-stepsize methods under certain circumstances. More progress can be expected from the density control developed recently for geometric integration and other methods (see, for example, [2], [6], [20]). However, such improvements seem not to be able to resolve the principal difficulty of the fixed-stepsize implementation of doubly quasi-consistent methods in the sense of the global

error control efficiency. To match a proper grid for a user-supplied accuracy condition we have to repeat the computation from the beginning of the integration interval. On the other hand, the local and true errors of doubly quasi-consistent schemes are almost the same. This means that recomputations from the starting point are not necessary in the new class of methods. We will address this point in a future paper. To implement our goal, we plan first to construct variable-stepsize doubly quasi-consistent peer methods. We will also look for numerical integration techniques of higher order that are suitable for practical use.

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